NEMO: General Release of a New Comprehensive Quantum Device Simulator

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Abstract. Device simulations are essential to explore new device designs, optimize performance, and analyze the underlying physics. Nanoelectronic devices pose a new challenge in this area since conventional drift-diffusion simulators are not applicable. **NEMO** (NanoElectronic MOdeling) is a new quantum device simulator based on a non-equilibrium Green's function formalism that simulates a wide variety of quantum devices, including RTDs, HEMTs, HBTs, superlattices, and Esaki diodes. Here we announce the general release of **NEMO** as a national resource freely available to the US scientific community. We will present **NEMO** calculations for InGaAs / AlAs and GaAs / AlAs RTD devices.

1. Introduction

Advances in epitaxial growth and device processing techniques have spurred development of heterostructure devices based on quantum confinement and resonant tunneling effects. As these devices transfer from the laboratory to commercial applications, accurate device simulations will be essential to optimize device performance, explore new device designs, and to understand the quantum effects that drive the transport process. Conventional simulators such as **PISCES** cannot analyze nanoelectronic devices without resorting to *ad hoc* models that do not include the underlying physics of the quantum transport.

To address this problem, we developed a general purpose 1-D quantum device simulator called **NEMO** (NanoElectronic MOdeling). Here we announce the general release of **NEMO** as a national resource available free of charge to the US scientific community and describe some of its features. We also give examples of NEMO calculations for InGaAs / AlAs and GaAs / AlAs RTD devices. Detailed discussion of the NEMO theory and its application to various devices are given in Refs. [1], [2], and references therein.

2. NEMO Features

NEMO uses a non-equilibrium Green's function algorithm that can incorporate any combination of potential, band structure, and scattering models. This approach has proven to be applicable to a wide range of device designs, numerically stable, and computationally efficient. Table 1 illustrates the some of the devices, material systems, and output options available in **NEMO**. Table 2 lists the potential, band structure, and scattering models.

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NEMO Features	Devices	Material Systems	Output Options
Variety of device designs	RTD	AlGaAs	Current
Long devices (> 100 nm)	HBT	InGaAs	Energy Bands
Large biases	HEMT	InAlAs	Band Profile
Temperature range 0 - 300 K	MOS	Silicon (MOS only)	Transmission Coefficient
	Esaki diodes		Energy Resonances
	Superlattices		Charge Density
			Resonant Wavefunctions
			Density of States

Table 1. A summary of features, device types, material systems, and output options modeled with **NEMO**.

Potential	Band Structure	Scattering
Thomas-Fermi	**Single-band effective mass**	**Single Band**
Hartree	**Multiple decoupled single bands**	Acoustic phonon
Hartree	**Non-parabolic single-band**	Polar optical phonon
w/ exchange correllation	**k•p 2-band**	Interface roughness
	sp^3s^* 10-band	Alloy disorder
	1^{st} nearest neighbor	**Multi-Band**
	2^{nd} nearest neighbor	Relaxation-time approx.
	spin-orbit coupling	in contact layers

Table 2. Models provided by **NEMO**. The user can mix any combination of these models to optimize calculation accuracy, execution time, and memory usage.

A major thrust of the **NEMO** project was to provide a user-friendly tool designed for both scientific and engineering applications. To achieve this flexibility and ease-of-use, graphical user interface (GUI) development was a major part of the **NEMO** effort. The **NEMO** GUI gives user as much control as possible over every aspect of the simulation and plots the calculation results in real-time. Some of the key **NEMO** GUI features include:

- Display and entry of all device, material, and simulation parameters.
- Default values provided for material and simulation parameters.
- Display of calculation results in 2-D, 3-D, and contour plots.
- Real-time band profile calculation with mouse-adjustable Fermi level.
- Plot Slicers to display slices of 3-D data sets.
- Plot Slicers Linker connects all Plot Slicers to a cursor on the I-V data.
- Library of example **NEMO** simulations.
- Band Structure tool to display energy bands and electron density vs. Fermi energy.
- Material parameter tool that displays material parameter equations and allows exploration of material properties vs. composition and temperature.
- Operates on HP-UX, Sun, and SGI with possible extension to DEC/Alpha and IBM/AIX platforms.

The Plot Slicer is particularly useful as it allows the user to review all of the calculation results and link them to a master slide bar connected to the I-V calculation. Figures 1 and 2 illustrate some of these graphical tools.

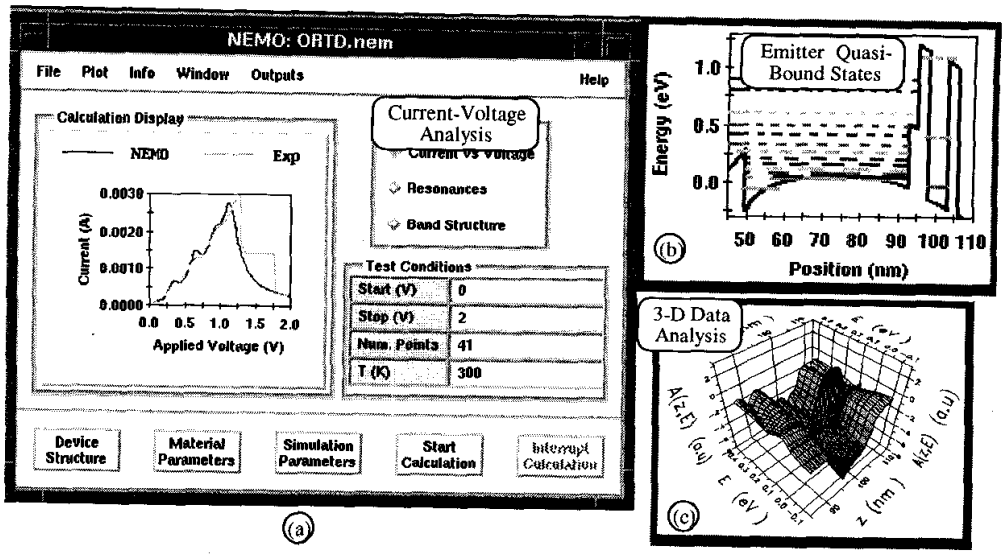

FIG. 1. Overview of several of **NEMO**'s interactive windows: (a) Main window compares a simulation of current vs. voltage for an optical resonant tunneling device (ORTD) to experimental data. The main window provides access to other tools used for the device design. (b) The energy band profile and resonance states calculated for the ORTD device. (c) 3-D display of the spectral function in the center of the ORTD.

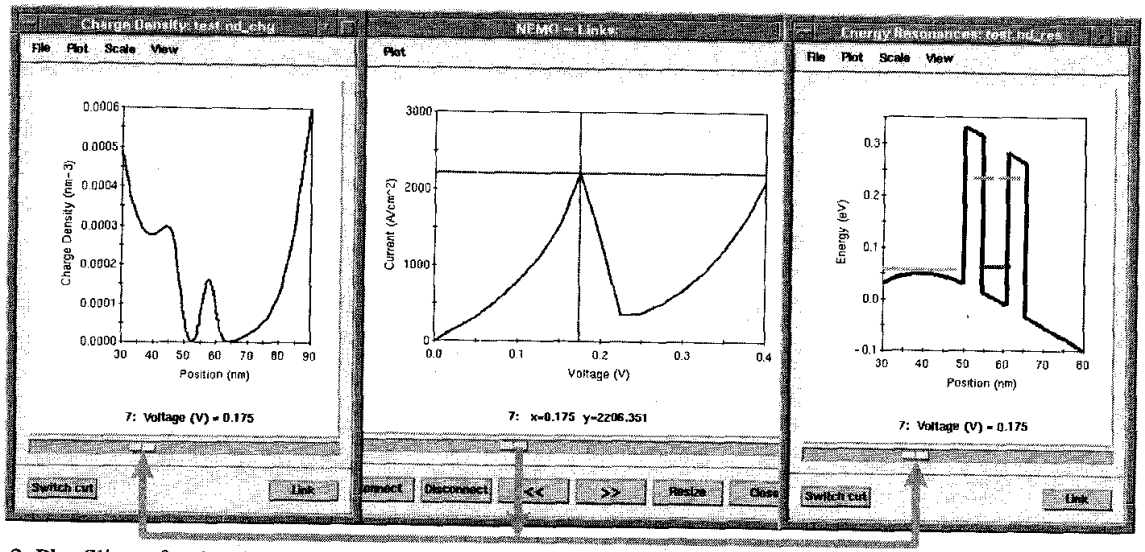

FIG. 2. Plot Slicers for the charge distribution (left) and band profile with energy resonances (right) linked to the current vs. voltage scan (center). The Link tool can couple all output graphs as a function of bias. Quick keys("<<" ">>") switch the scroll bar between maximum and minimum extrema in the I-V data.

3. Simulation Examples

As an example, we illustrate RTDs built in two different material systems. The first device shown in the inset of Fig. 3 is an $In_{0.53}Ga_{0.47}As$ / $In_{0.52}Al_{0.48}As$ RTD operating at room temperature. **NEMO** employs a 10-band sp^3s^* bandstructure model to determine the non-parabolic E(**k**) dispersion for the InGaAs and InAlAs conduction bands. A numerical integration method calculates the transmission

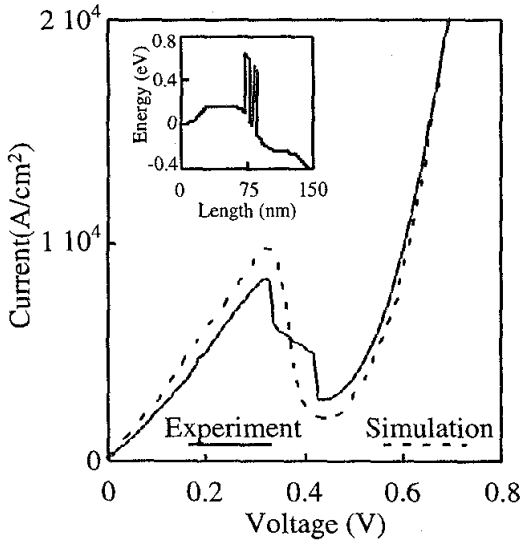

FIG. 3. Current vs. voltage characteristic of an $In_{0.53}Ga_{0.47}As$ / $In_{0.52}Al_{0.48}As$ resonant tunneling diode (see the conduction band edge in the inset) at room temperature calculated in a 10-band model with full-band integration and no scattering in the central RTD region.

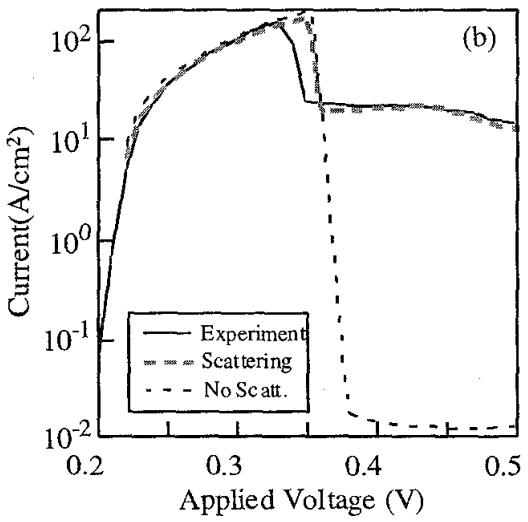

FIG. 4. Current vs. voltage characteristic of an GaAs / AlAs resonant tunneling diode at a temperature of 4.2 K. A phonon peak is visible in the valley current region.

including the dependence on transverse momentum. The predicted valley current and peak-to-valley ratio show good agreement with the experiment even though the simulation neglects scattering effects in the central quantum region (a relaxation-time approximation accounts for scattering in the reservoirs outside the central region). This indicates that thermionic emission through the first excited quantum well state dominates the room temperature valley current.

The second device is a GaAs / AlAs RTD measured at T=4.2K. The **NEMO** simulation shows that a polar-optical-phonon assisted tunneling process dominates the valley current (Fig. 4). If we neglect polar optical phonon scattering, the calculated valley current is too low by 3 orders of magnitude.

4. Conclusion

In conclusion, **NEMO** is a comprehensive, versatile, and user-friendly quantum device modeling tool with predictive capabilityfor a wide range of devices and operating conditions. The general release is slated for the December 15 of 1997 at which time it will be available to any interested domestic industrial and educational facilities. To obtain NEMO, contact Gerhard Klimeck at Raytheon TI Systems, phone 972-995-5510, email gekco@ti.com.

References

[1] Klimeck G, Lake R, Bowen R C, Frensley W R, and Moise T S, "Quantum Device Simulation with a generalized tunneling formula", 1995 *Appl. Phys.* Lett. 67(17) 2539-41.

[2] Lake R, Klimeck G, Bowen R C, Jovanovic D, "Single and Multi-Band Modeling of Quantum Electron Transport Through Layered Semiconductor Devices", 1997 *J. Appl. Phys.* 81(12): 7845-69.